REMARKS

Claims 37-72 were examined, with claims 1-18 and 25-36 withdrawn from consideration. The Examiner rejected claims 37-72. Applicants have herein cancelled claims 1-18 and 25-36, and amended claims 37 and 55. Support for the amendments can be found throughout the Specification as originally filed, *e.g.*, among others, paragraphs [0007] – [0009] and [0029] – [0037] of the publication of the present application, U.S. 2004/0148149. In paragraph [0007], for example, the Specification notes "the invention features a method for designing a metal ion ... including the steps of a) building a *metal ion molecule* having a center atom and a dummy atom" (emphasis added). Paragraph [0009] notes that the metal ions include "zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, magnesium, and any other main group and/or transition metal ion." In addition, in paragraph [0030], the Specification states that "the Zn^{2+} ion can be replaced with a *five-atom molecule* referred to herein as a tetrahedral zinc *molecule*" (emphasis added). Moreover, paragraph [0031] states that "[a] tetrahedral zinc *molecule* having a tetrahedral configuration has five atoms. One atom is located at the center of the zinc molecule. This center atom is assigned the total size of the molecule . . .. The remaining four atoms are covalently bound to the center atom and are referred to as dummy atoms. . . . [A] dummy atom is basically a point charge. . . . In particular, it is advantageous to assign a fraction of the total charge of the ion to each dummy atom" (emphasis added). Finally, in paragraph [0035], the Specification states "[i]t may be helpful to adjust the van der Waals radius of the center atom of the zinc tetrahedron molecule (*or other transition metal polyhedron molecule*)" (emphasis added). Accordingly, no new matter has been added.

Applicants thank the Examiner for the courtesy of a telephonic interview on October 26, 2007. As noted in the Examiner's Interview Summary dated October 30, 2007, possible amendments to the claims were discussed to overcome the 35 U.S.C. §§ 101 and 112, second paragraph rejections.

In view of the amendments and the remarks herein, Applicants respectfully request reconsideration and allowance of the pending claims.

Rejections under § 101

The Examiner rejected claims 37-72 as directed to non-statutory subject matter. Applicants respectfully disagree with respect to the claims as currently amended. It is believed that the present amendments render the claims useful, concrete, and tangible, as the recited methods include, among other limitations, generating a representation or simulation *for observation by a user on a display*. Thus, the claims represent statutory subject matter. Withdrawal of the rejections is respectfully requested.

Rejections under 35 U.S.C. § 112, second paragraph

The Examiner rejected claims 37-72 as allegedly being indefinite. In particular, the Examiner alleged that it was unclear how a monoatomic ion that can include a center atom and a dummy atom could be polyatomic and monoatomic at the same time; and further alleged that proper antecedent basis for certain terms was absent.

Applicants respectfully disagree with respect to the claims as currently amended. First, Applicants note that the Examiner's rejections regarding proper antecedent basis for the term "metal ion" in claims 37 and 55 has been rendered moot by the present amendments. Withdrawal of the rejections is respectfully requested.

Secondly, present independent claims 37 and 55 recite, respectively, methods whereby a representation or simulation of a monoatomic metal ion *as a metal molecule* is performed. In these claims, the recited metal molecule comprises a plurality of atoms comprising a center atom and one or more dummy atoms, where the center atom has a van der Waals radius greater than zero, where the center atom is covalently linked to the one or more dummy atoms, and where each dummy atom has a positive charge. Applicants respectfully assert that the presently amended claims are now definite and clear, as the representation of a metal ion as a *metal molecule* encompasses the use of multiple (*i.e.*, a plurality of) atoms. Accordingly, withdrawal of the rejections is respectfully requested.

Finally, with respect to the § 112, second paragraph rejections of claims 52-53 and 70-71, Applicants note that their prior Amendment dated June 15, 2007 cancelled the positive and

negative charge limitation, represented by the "±" symbol, by striking through it, and amended the claims to recite only the limitation "+" by underlining the "+" symbol. Applicants note that a "+" symbol underlined looks similar to the "±" symbol, and believe that is the basis for the Examiner's rejection. Applicants refer the Examiner to the prior amendment for confirmation that the Applicants had indeed deleted the "±"symbol (via strikethrough) and added (via underlining) only the "+" symbol. The claims as set forth above reflect this amendment. Accordingly, withdrawal of the rejections is respectfully requested.

CONCLUSIONS

Applicants respectfully assert that all claims are in condition for allowance, which action is hereby requested. The Examiner is invited to telephone the undersigned to expedite prosecution.

No fee is believed due. Please apply any charges or credits to deposit account 06-1050.

Respectfully submitted,

Date: 12/7/07

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